

Configuration Space for Random Walk Dynamics¹

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Abstract

Applied to statistical physics models, the random cost algorithm enforces a Random Walk (RW) in energy (or possibly other thermodynamic quantities). The dynamics of this procedure is distinct from fixed weight updates. The probability for a configuration to be sampled depends on a number of unusual quantities, which are explained in this paper. This has been overlooked in recent literature, where the method is advertised for the calculation of canonical expectation values. We illustrate these points for the $2d$ Ising model. In addition, we prove a previously conjectured equation which relates microcanonical expectation values to the spectral density.

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The performance of a numerical simulation depends on the chosen weight factors. Hence, some attempt should be made to optimize them for the problem at hand. The weight function of canonical MC simulations is $\exp(-\beta E)$, where E is the energy of the configuration to be updated and β is the inverse temperature in natural units. The Metropolis algorithm and other methods generate canonical configurations (*i.e.* the Gibbs ensemble) through a Markov process. It has been expert wisdom [1] for quite a while and became widely recognized in recent years that MC simulations with a-priori unknown weight factors are also feasible and deserve to be considered, for a concise recent review see [2]. For instance, weighting (in a certain energy range) with the inverse spectral density $1/n(E)$ has turned out to be of practical importance. Examples are calculations of interfacial tensions for first order phase transitions, where improvements of many orders of magnitude were obtained. Instead of the energy other thermodynamic variables can be considered as well, *e.g.* [3]. To be definite, we focus on the energy.

MC simulations with a-priori unknown weight factors require an additional step, not encountered in canonical simulations: A working estimate of the weight factors needs to be obtained first. Quite efficient recursive methods have been developed for this purpose [4]. Still, the question suggests itself whether one can possibly bypass the first step and develop methods which sample broad energy distributions right away. Indeed, it is possible to design updates such that a RW in some cost function is generated [5] and the energy of a statistical physics model can be chosen as cost function. Unfortunately (as already noted in [5]) the connection to the desired canonical expectation values is apparently lost. Nevertheless, it appears to be worthwhile to investigate properties of the thus generated configurations. In particular, some details are subtle and, besides the origin of the method, ignored in recent literature [6].

We consider generalized Ising models in d dimensions, described by the energy function

$$E = - \sum_{ij} J_{ij} s_i s_j \quad (1)$$

where the sum is over nearest neighbors and the exchange coupling constants J_{ij} as well as the spins s_i, s_j take the values ± 1 . The Ising ferromagnet is obtained with $J_{ij} \equiv 1$. Other special cases are the Ising anti-ferromagnet, frustrated Ising models and spin glasses. We consider a configuration of N spins and choose periodic boundary conditions. Under flip of a single spin the energy can change by the following increments

$$\Delta E_i = 4i \text{ with } i = -d, \dots, -1, 0, 1, \dots, d. \quad (2)$$

In the following we use i to label Flip Groups (FGs) of spins. We define now numbers

$$N_i \text{ with } i = -d, -d+1, \dots, d-1, d \text{ and } \sum_{i=-d}^d N_i = N \quad (3)$$

to partition the configuration of N spins with respect to the FGs. Namely, N_i denotes the number of spins which, when flipped, change the energy by $\Delta E = 4i$. In the following N_i is referred to as Flip Group Magnitude (FGM). The random cost algorithm [5] achieves a RW in energy by flipping spins with suitable probabilities related to FGs. Let P_i be the probability for picking and flipping a spin in the FG labeled by i . A RW in E is obtained whenever the equation

$$\sum_{i=1}^d i (P_i - P_{-i}) = 0 \quad (4)$$

holds, because the expectation value of energy changes $\overline{\Delta E}$ becomes then zero. It should be noted that P_0 does not enter this equation and can be chosen at will. Besides, equation (4) does not fix the other probabilities either, but allows considerable freedom concerning their further design. Before we come to this, let us note that N_i has to be greater than zero for at least one $i \geq 1$ and one $i \leq -1$. Otherwise, a RW can no longer be achieved. This

latter difficulty happens in a local minimum or maximum of the system and, by whatever additional rule, one or more spins have to be flipped before the RW simulation can continue. In the following we assume that the noted $N_i > 0$ condition is fulfilled.

Solutions to (4) are easily found, the following is given in [5]. We define

$$\Delta E^+ = \frac{1}{N^+} \sum_{i=1}^d N_i \Delta E_i \quad \text{and} \quad \Delta E^- = \frac{1}{N^-} \sum_{i=1}^d N_{-i} \Delta E_{-i} \quad (5)$$

where

$$N^+ = \sum_{i=1}^d N_i \quad \text{and} \quad N^- = \sum_{i=1}^d N_{-i} . \quad (6)$$

In the same way, we define

$$P^+ = \sum_{i=1}^d P_i \quad \text{and} \quad P^- = \sum_{i=1}^d P_{-i} . \quad (7)$$

I.e. P^+ is the probability to pick any of the spins from the $i \geq 1$ FGs and P^- is the probability to pick any of the spins from the $i \leq -1$ FGs. Finally, assume that within those FGs the spins are picked with uniform probability, with $p^+ = P^+/N^+$ for $i \geq 1$ and with $p^- = P^-/N^-$ for $i \leq -1$. The RW equation (4) is then implied by the condition

$$-P^- \Delta E^- = P^+ \Delta E^+ . \quad (8)$$

Choosing an arbitrary probability P_0 , the probabilities P^+ and P^- follow immediately from this equation and the normalization condition $P_0 + P^+ + P^- = 1$. Another way [6] to implement (4) is to choose a spin at random and to reject the flip with the appropriate probability, then counting the configuration at hand again. Here we stay with (8).

It follows from equations (3) and (4) that every such algorithm samples with weights which depend on the FGs

$$w = w(N_{-d}, N_{-d+1}, \dots, N_{d-1}, N_d) . \quad (9)$$

For configurations at a fixed energy E the implication of this equation is that the RW algorithm weights them differently depending on the FGM partition, whereas canonically all these configurations have the same weight. In the following we illustrate this point for the $2d$ Ising ferromagnet.

We have performed canonical as well as RW simulations for $2d$ Ising models on $N = L^2$ lattices with periodic boundary conditions. For the RW updating we used $P_0 = 0.2$ and did a random flip, once the energy minimum was reached. At large energy we imposed a cut-off [7] at $E = 0$, by replacing RW with random (canonical $\beta = 1/(k_B T) = 0$) updating for $E > 0$. To avoid getting lost in a flood of data, we focus on a single energy. After gaining some experience $E/N = -1$ with canonical simulations at $\beta = 0.38$ turned out to be a reasonable choice ($\overline{E}(\beta = 0.38)/N \approx -1$). This value is in the disordered phase for β below the Curie point at $\beta_c = 0.5 \ln(1 + \sqrt{2}) = 0.4406 \dots$. This correspond to a configuration space region far away from the energy minimum $E/N = -2$ or the upper energy bound $E/N = 0$ imposed on the RW simulation. The lattice sizes used are $L = 4, 10, 20, 40$ and 80 . For each case we generated a statistics of $20 \times 100,000$ sweeps through the lattice and calculated error bars with respect to twenty bins. For $L = 4$ we also obtained exact results by simply counting through all 2^{16} configurations and convinced ourselves that the canonical simulation agrees (within very small statistical errors) with these exact results, whereas the RW simulation shows already considerable deviations.

Let us focus on the microcanonical average values \overline{N}_i/N . For the $L = 80$ lattice table 1 collects results from the canonical as well as from the RW simulation. Although over-all small, in case of \overline{N}_{-2}/N the discrepancy is about a factor of two and for all FGs the difference between the canonical and the RW values clearly exceed the error bars. In the average most spins, about 39%, are found in the FG with number $i = 2$. Hence, we have the best statistics for this FG and choose it to demonstrate a few more details. Although the discrepancy

between the \overline{N}_2/N values of the table appears quite small, there are considerable differences when we look at the distribution of N_2 . To correct for the expected (non-critical) finite size behavior, we define the quantity

$$n = L^{-1} (\overline{N}_2 - N_2) . \quad (10)$$

Figure 1 shows the canonical and the RW histograms $h_2(n)$, all normalized to

$$L^{-1} \sum_n h_2(n) = 1 .$$

Error bars are negligible on the scale of this figure. The canonical histograms for the different lattice sizes collapse nicely into one curve, whereas the finite size behavior of the RW histograms fails to reproduce this behavior. The RW histograms are far too broad and the peak height decreases with lattice size, implying that the discrepancy to canonical simulation increases with lattice size. The $L = 4$ data do not fit into the scale of this figure. As there are only four non-zero entries, we collect them in table 2.

By taking averages, the dependence on the FGMs appears to be washed out. This is obvious for the average \overline{N}_i/N values reported in table 1 and claimed [6] to be true for thermodynamic quantities like the energy and the specific heat. The latter quantities were calculated from the spectral density $g(E)$ which, in turn, was determined from the conjectured equations

$$\overline{N}_i(E) g(E) = \overline{N}_{-i}(E + \Delta E_i) g(E + \Delta E_i) . \quad (11)$$

In appendix A we give a mathematical proof of these equations. From this it follows that the $\overline{N}_i(E)$ are microcanonical averages and *not* averages accumulated during the RW, as stated in [6]. Only canonical, microcanonical or other simulations which give equal weights to distinct configurations at the same energy will converge towards the correct $\overline{N}_i(E)$ values for this equation. A rigorous calculation of the spectral density $g(E)$ from RW data is not possible, because the RW weights depend on the FGMs (3) [8].

For the $L = 80$ lattice table 1 lists RW and canonical expectation values for the $\overline{N}_i(E)$ at $E/N = -1$. As the differences are not too large, it is plausible that some RW and canonical results can be in qualitative agreement with one another. However, it is obvious that the dependence of the RW configurations weights (9) on the FGM partition $\{N_i\}$ enter the Markov process. Even small deviations from the canonical weights may amplify, because they enter multiplicatively through each transition step. If the RW method is nevertheless used to estimate canonical expectation values, uncontrolled errors result with no guarantee that they will be negligible when it really matters (Murphy's law).

A simulation is normally already subject to finite size and other difficult to control approximations. Certainly, one would not like to build a large scale numerical investigation on a method which introduces an additional bias. The question arises, whether the weight dependence (9) could eventually be controlled rigorously. Due to the large number of partitions of the total number of spins N into FGMs (3) the prospects for this do not look particularly good, but it may be worthwhile trying. Finally, we like to emphasize that the RW approach remains a competitive method for the purpose it was originally [5] designated for, namely to find good energy minima for optimization problems and systems with conflicting constraints.

Appendix A

Here we prove equation (11) for the d -dimensional generalized Ising mode on a lattice with periodic boundary condition. Let K denote a spin configuration at energy E . By definition

$$\overline{N}_i(E) = \frac{1}{g(E)} \sum_K N_i(K)$$

holds. We introduce $E' = E + \Delta E_i$ and label spin configurations at energy E' by K' . Then

$$\overline{N}_i(E') = \frac{1}{g(E')} \sum_{K'} N_i(K')$$

and equation (11) becomes equivalent to

$$\sum_K N_i(K) = \sum_{K'} N_{-i}(K') . \quad (12)$$

Equation (12) is shown as follows. We label spins in a fixed configuration by $s_n(K)$ where $n = 1, \dots, N$ and N is the (fixed) total number of spins. In this way each single spin is uniquely identified. The same is true for spins $s_m(K')$ in the configurations at energy E' . Assume now, spin $s_{n_1}(K_1)$ is in flip group i and we flip it. It becomes a spin $s_{m_1}(K'_1)$ in the flip group $-i$ at energy E' . No other spin, say $s_{n_2}(K_2)$ with at least $n_2 \neq n_1$ or $K_1 \neq K_2$, will be mapped on $s_{m_1}(K'_1)$. The reason is: we can flip the spin $s_{m_1}(K'_1)$ back and it will map precisely onto the original configuration and spin, *i.e.* become $s_{n_1}(K_1)$. The same argument applies when we flip an arbitrary spin from flip group $-i$ at energy E' . Together this proves: spins in the flip groups with magnitudes $N_i(K)$ and $N_{-i}(K')$ are in on-to-one correspondence and, hence, equation (12) is true.

References

- [1] G.M. Torrie and J.P. Valleau, J. Comp. Phys. **22**, 187 (1977).
- [2] B.A. Berg, in: *Multiscale Phenomena and Their Simulation*, Proceedings of the International Conference, Bielefeld, Sept. 30 – Oct. 4, 1996, eds. F. Karsch, B. Monien, and H. Satz (World Scientific, Singapore, 1997), pp. 137-146.
- [3] B.A. Berg, U. Hansmann, and T. Neuhaus, Z. Phys. **90**, 229 (1993); N.B. Wilding and M. Müller, J. Chem. Phys. **102**, 2562 (1995); W. Janke and S. Kappler, Phys. Rev. Lett. **74**, 212 (1995).
- [4] B.A. Berg, Nucl. Phys. B (Proc. Suppl.) **63A-C**, 982 (1998); J. Stat. Phys. **82**, 323 (1996).

- [5] B.A. Berg, Nature **361** (1993) 708; Comp. Phys. Commun. **98** (1996) 35.
- [6] P.M.C. de Oliveira, T.J.P. Penna and H.J. Herrmann, Braz. J. Phys. **26** (1996) 677; Europ. Phys. J. **B1** (1998) 205. After submitting our paper we were informed about one further reference: P.M.C. de Oliveira, Int. J. Mod. Phys. **C 9** (1998) 497.
- [7] Without this cut-off the RW would extend all the way to $E/N = +2$, where a method of return has then to be imposed anyway. In our RW simulations slowing down (measured in CPU time) is with the square (or worse) of the length of the RW. Hence, without this cut-off CPU time consumption would increase by at least a factor of four.
- [8] For the 1d Ising model RW and microcanonical expectation values for $\overline{N}_i(E)$ may agree due to the trivial character of the model: It has only one FG for $i \geq 1$ and one FG for $i \leq -1$.

Tables and Figure Captions

i	-2	-1	0	1	2
CS	0.018853 (03)	0.072752 (04)	0.187630 (07)	0.331070 (11)	0.389694 (09)
RW	0.034282 (26)	0.057936 (19)	0.169412 (57)	0.350240 (43)	0.388130 (55)

Table 1: Average Flip Group Magnitudes \overline{N}_i/N , $i = -2, \dots, 2$ as obtained for the Canonical Simulation (CS) versus the Random Walk (RW) simulation on a 80×80 lattice. Error bars are given in the parenthesis and apply to the last two digits.

Figure 1: Canonical and RW histograms $h_2(n)$ at $E/N = -1$ with n given by (10). All the canonical histograms collapse onto the highest curve. The RW histograms follow in the order $L = 10, 20, 40$ and 80 from up to down.

n	-1.5276	-0.5276	-0.0276	0.4724
N_2	0	4	6	8
Exact	$32/424 =$	$192/424 =$	$1088/424 =$	$384/424 =$
Exact	0.07547...	0.45283...	2.56603...	0.90566...
CS	0.0759(11)	0.4543(35)	2.5672(43)	0.9026(31)
RW	0.2216(08)	0.5471(07)	2.3080(11)	0.9233(10)

Table 2: The $h_2(n)$ histogram results for the $L = 4$ lattice (on this lattice there are 424 configurations at $E/N = -1$).

